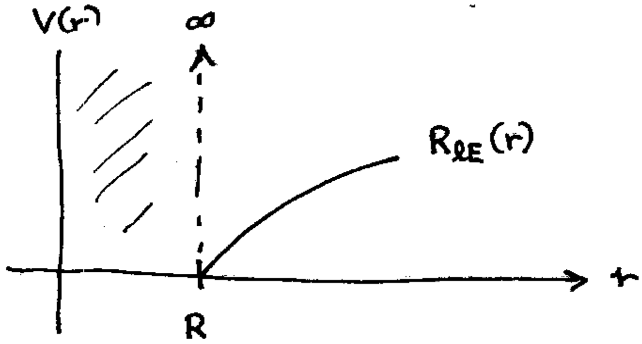
We continue with central force scattering. First we look at an example, namely, hard-sphere scattering. In this case the potential $V(r)$ is



$$V(r) = \begin{cases} \infty, & r < R \\ 0, & r > R. \end{cases}$$

don't confuse $\begin{cases} R = \text{radius of sphere} \\ R_{\ell E}(r) = \text{wave fn.} \end{cases}$

The wave fn $R_{\ell E}(r)$ must vanish at $r = R$. Solution for $r > R$ is free particle,

$$R_{\ell E}(r) = A j_\ell(kr) + B y_\ell(kr) \qquad (r > R)$$

but bdry conditions imply

$$R_{\ell E}(R) = 0 = A j_\ell(kR) + B y_\ell(kR),$$

or

$$\frac{B}{A} = -\frac{j_\ell(kR)}{y_\ell(kR)}.$$

Phase shift δ_ℓ is determined from asymptotic form,

$$R_{\ell E}(r) \underset{r\to\infty}{\sim} \frac{A \sin(kr - \ell\pi/2) - B \cos(kr - \ell\pi/2)}{kr}$$

using asymptotic forms of j_ℓ, y_ℓ fns. This can be written,

$$= C \, \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr},$$

where

$$\left.\begin{aligned} A &= C\cos\delta_\ell \\ B &= -C\sin\delta_\ell \end{aligned}\right\}$$

or

$$\frac{B}{A} = -\tan\delta_\ell$$

or

$$\boxed{\tan\delta_\ell = \frac{j_\ell(kR)}{y_\ell(kR)}}$$

This gives phase shifts δ_ℓ (a property of wave field at $r\to\infty$) in terms of wave fns at $r=R$ (small r). Look at limiting cases.

Case I. $kR \ll 1$. Here we can use small argument limits of j_ℓ, y_ℓ (see Eqs. 14.26-14.27). Then

$$\tan\delta_\ell = \frac{(kR)^\ell}{1\cdot 3\cdots(2\ell+1)}\cdot\frac{-(kR)^{\ell+1}}{1\cdot 3\cdots(2\ell-1)} = -\frac{(kR)^{2\ell+1}}{[(2\ell-1)!!]^2(2\ell+1)}$$

$$= -\frac{(kR)^{2\ell+1}}{[(2\ell-1)!!]^2(2\ell+1)}.$$

If $kR \ll 1$, then $\tan\delta_\ell$ is small for all ℓ, and $\tan\delta_\ell \approx \delta_\ell$. Also, δ_ℓ is a strongly decreasing fn. of ℓ, so $\ell=0$ term is most important. This is an example of S-wave scattering, the scattered wave is isotropic and $d\sigma/d\Omega$ is indep. of θ. As for δ_0, it is

$$\delta_0 = -kR.$$

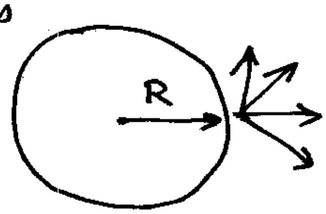
Keeping only $\ell=0$ term, we have

$$f(\theta) = -R$$

$$\frac{d\sigma}{d\Omega}(\theta) = |f|^2 = R^2, \qquad \boxed{\sigma = 4\pi R^2}$$

The total cross section is $4\times$ the geometrical cross section of the sphere, which is the ~~total~~ <u>classical</u> ~~crosssection~~ cross section πR^2. We do not expect the quantum cross section to agree with the classical when $kR \ll 1$, because this is the long wavelength limit, $\lambda \gg R$. We expect to see classical results when $\lambda \ll R$, that is, $kR \gg 1$.

<u>Case II</u>. $kR \gg 1$. In this case many terms contribute to the partial wave expansion of $f(\theta)$. We can see why by considering a classical picture, in which we stand on the surface of the sphere of radius R, and ~~fire~~ shoot particles of energy $E = p^2/2m$ in various directions. What is the maximum angular momentum L_{max} these particles can have? It is when the momentum $\vec{p}$ is $\perp$ to the radius $\vec{r}$, maximizing



$|\vec{L}| = |\vec{r}\times\vec{p}| = Rp$.

Interpreting $L_{max} = Rp$ in quantum mechanics, we set $L_{max} = l_{max}\hbar$ and $p = \hbar k$, or $l_{max}\hbar = \hbar(kR)$, or

$$\boxed{l_{max} = kR.}$$

This argument suggest (correctly) that when $kR \gg 1$, the partial wave series is dominated by terms out to $l = l_{max}$, which fall off rapidly after that.

Also, for the phase shifts, we can use the asymptotic forms (14.28)–(14.29), which are valid for $\rho = kR \gg l$, ie, $l \ll l_{max}$. In fact they work pretty well up to $l \approx l_{max} = kR$. So we have in this range of l values,

$$\tan\delta_l = -\frac{\sin(kR - l\pi/2)}{\cos(kR - l\pi/2)} = -\tan(kR - l\pi/2),$$

or

$$\delta_l = -(kR - l\pi/2).$$

δ_l increases by $\pi/2$ when l increases by 1. Therefore

$$\sin\delta_{l+1} = \sin(\delta_l + \pi/2) = \cos\delta_l$$

or

$$\sin^2\delta_{l+1} + \sin^2\delta_l = 1.$$

So in the series,

$$\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l,$$

$\sin^2\delta_l$ has the average value of $\frac{1}{2}$, and the series approximately sums to

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{l_{max}}(2l+1)\cdot\frac{1}{2} = \frac{4\pi}{k^2}(l_{max}+1)^2\cdot\frac{1}{2}$$

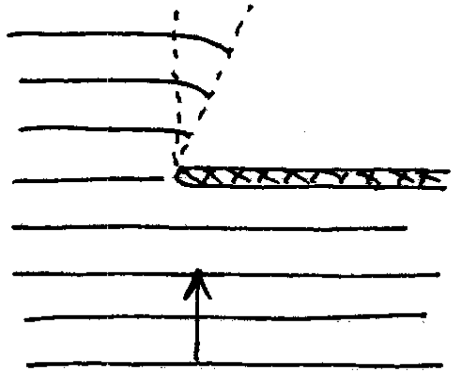
or

$$\boxed{\sigma = 2\pi R^2} \quad \text{(High } k \text{ limit).}$$

Here we ignore the difference between l_{max} and $l_{max}+1$. At high energy, the total cross section is twice the classical value.

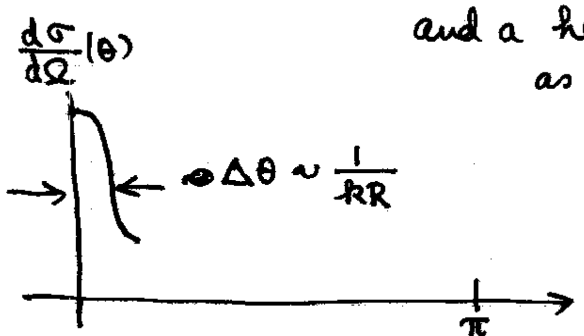
This is a paradox, since we might have expected to get the classical cross section when $kR \gg 1$, ie., $\lambda \ll R$.

The reason why we do not is because of diffraction. Diffraction is the bending of a wave as it passes around an obstacle.



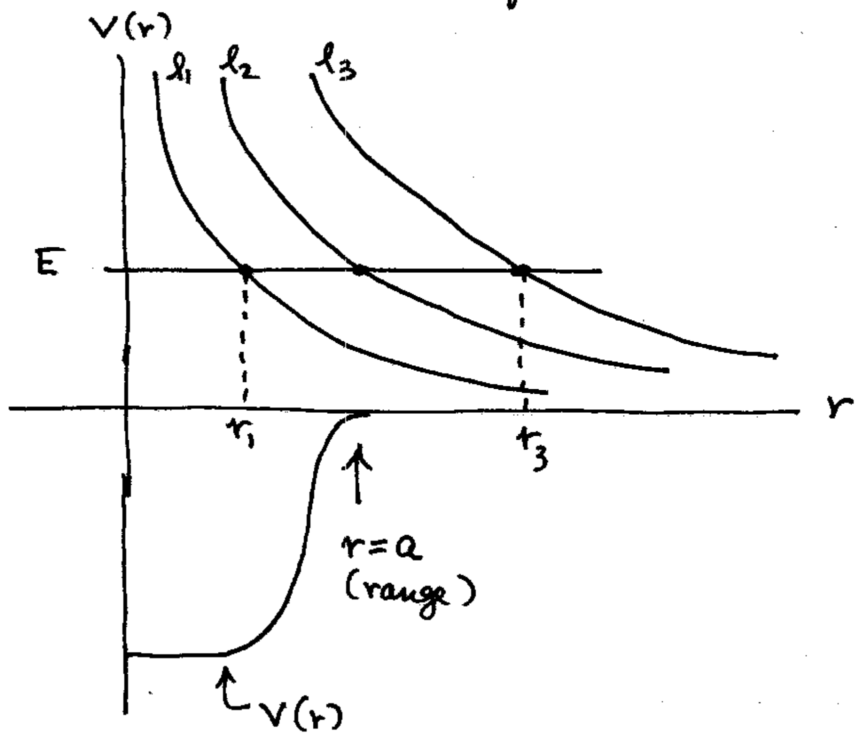
The wave bends toward the shadow region, partially filling it in. Diffraction can be understood in terms of the uncertainty principle. Speaking of quantum waves, restricting the transverse position of the particles gives them a transverse component to their momentum. These particles have been scattered, that is, their momentum has been altered.

As $k \to \infty$ (or $\lambda \to 0$), the angle of diffraction decreases. In that sense, things look more classical. But the total flux of scattered particles (by diffraction) remains constant. Thus, as $\lambda \to 0$, $\frac{d\sigma}{d\Omega}(\theta)$ starts to look more like a δ-fn around $\theta = 0$, the ~~dir~~ forward direction. The peak has a width $\sim \frac{1}{kR}$ and a height that grows as $(kR)^2$.



For $\theta \neq 0$, the limit $\lambda \to 0$ does produce the classical $\frac{d\sigma}{d\Omega}(\theta)$; but right around $\theta = 0$ diffraction scattering contributes a total of πR^2, making the total $\sigma = 2\pi R^2$.

Now we look at general properties of the phase shifts δ_ℓ. We consider first a short range potential $V(r)$, defined as one that goes to 0 exponentially or faster beyond a radius $r = a$, defined as the range of the potential. Potentials in nuclear physics have this property, with a on the order of a few $\times 10^{-13}$ cm. Here is a sketch in the case of an attractive potential:



Also sketched are 3 centrifugal potentials, with $l_1 < l_2 < l_3$. Also sketched is an energy E and its intersections with the 3 centrifugal potential curves, at locations r_1 and r_3 for curves l_1 and l_3. These points r_1 and r_3 are the turning points for energy E of a <u>free</u> particle of the given l. That is, the turning points are computed ignoring the true potential.

As For point r_3, it falls well outside the range a of the true potential, so for $r \geq r_3$ the total potential (centrif + true) is approximately the same as the centrifugal potential. A classical particle coming in on centrifugal potential curve l_3 would hit the turning point at r_3 and reflect back, without ever sensing the true potential. Also r_3 is approximately the turning point for the total effec. potential, since the true potential is small for $r \geq r_3$.

Thus the WKB solution for energy E and $l = l_3$ must look almost the same as that of a free particle, and the asymptotic phase shift δ_l, which is measured relative to the free particle phase shift, must be very small.

The quantum wave function does know about the true potential $V(r)$ because it can tunnel through the classically forbidden region and reach the region where $V(r)$ is not small. But tunneling is an exponentially decreasing function of the tunneling action, so we expect δ_l to decrease exponentially as l increases, $l \geq l_3$.

An exception to this is resonance scattering, which we discuss later.

For $l = l_1$, the turning point (in the centrifugal potential only) is r_1, which lies in the region where the true potential is large. So r_1 is not a good approximation to the turning point in the total effective potential, and the asymptotic phase shift is not well approximated by the free particle result. That is, δ_l is not small. The phase shift is only defined modulo π, so "not small" means, of order unity. But for $l = l_1$, the contribution to the partial wave expansion will be significant.

In between l_1 and l_3 there is some l value, call it l_{cutoff}, where the turning point in the centrifugal potential is approximately the range of the true potential a. We find the value $l = l_{cutoff}$ by setting

$$\frac{l(l+1)\hbar^2}{2ma^2} = E = \frac{\hbar^2 k^2}{2m},$$

or

$$\boxed{l_{cutoff} = ka}$$

where we replace $l(l+1)$ by l^2 since it is only an estimate.

We conclude that for short range potentials of range a, partial waves with $l < l_{cutoff}$ contribute significantly to the scattering amplitude, while those with $l > l_{cutoff}$ make only a small contribution, in fact δ_ℓ and hence the coefficients in the partial wave expansion decrease exponentially with ℓ when $\ell > \ell_{cutoff}$.

In atomic physics, power law potentials are more common. For example, neutral atoms interact via the dipole-dipole interaction, which falls off as $\frac{1}{r^6}$. In this case, one can show that δ_ℓ also decreases as an inverse power of ℓ for large ℓ.

Return to short range potentials. For the case $ka \ll 1$ (low energy), the scattering amplitude is dominated by a single term $\ell = 0$. This is <u>s-wave scattering</u>, which holds in most potentials if the energy is low. The scattering is isotropic, and is described by a single parameter δ_0. The scattering amplitude and cross section are

$$f(\theta) = \frac{1}{k} e^{i\delta_0} \sin\delta_0 \quad = \text{indep. of } \theta,$$

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{\sin^2\delta_0}{k^2},$$

$$\sigma = \frac{4\pi}{k^2} \sin^2\delta_0.$$

Low energy scattering is important in Bose-Einstein condensates (BEC's). BE condensation occurs when the temperature is low enough that the de Broglie wavelength of the atoms is comparable to the inter-atomic separation. But BEC gasses are low density, so the inter-atomic separation is much larger than the atomic size, which is roughly the range of the interaction between the atoms. Thus $kR \ll 1$. Atom-atom scattering in BEC's is important in limiting the lifetime of the condensate, which is not truly an ideal gas. BEC's are quite different (and easier) than systems like liquid helium, which also exhibit condensation of a kind, but where the atoms are touching one another.

Another example of s-wave scattering is neutron scattering from nuclei in matter at sufficiently low energy. Here "low energy" means less than several MeV, which makes the neutron λ larger than the size of a nucleus (it depends somewhat on the nucleus). Thus neutrons from a fission reactor satisfy this condition reasonably well, and after they have been slowed down by collisions with matter, the condition $ka \ll 1$ is very well met. Then we have s-wave scattering.

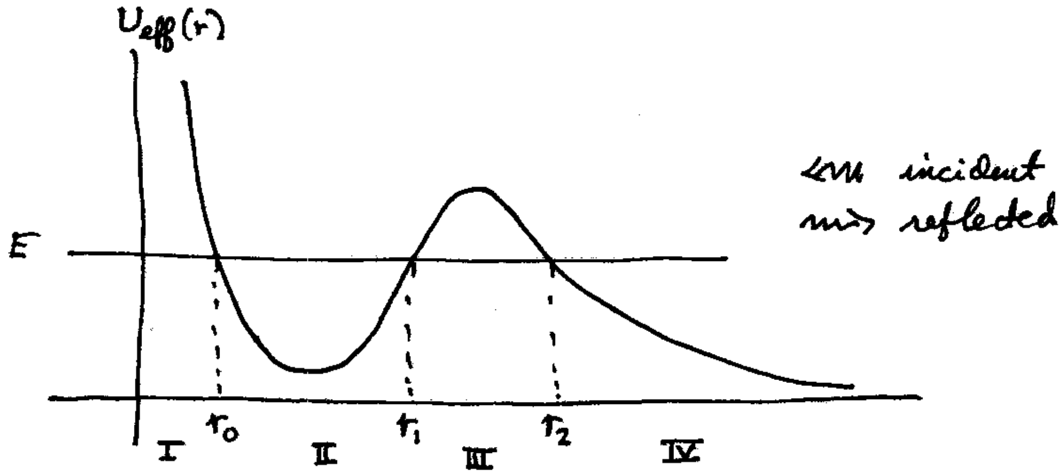
S-wave scattering is described by a single parameter, the phase shift δ_0 (which however is a function of E, but in many applications only the value at $E=0$ is important). Thus any other potential with the same δ_0 will have the same effects, insofar as low energy scattering is concerned. Often a convenient choice is a δ-function potential, with a strength chosen to make δ_0 come out right. This partly explains the popularity of δ-fn potentials in theoretical models.

At the high energy limit $ka \gg 1$, many partial waves contribute, and the partial wave expansion will require numerical work or analytical summation techniques to be useful. The number of terms is $\simeq l_{cutoff} \simeq ka$.

It is possible to make statements about $f(\theta)$ or $\frac{d\sigma}{d\Omega}(\theta)$, based on the general properties of the phase shifts. The series are Legendre polynomial expansions, but the principles are very similar to those for Fourier series. If the series is dominated by terms $l \lesssim l_{cutoff}$, then the minimum size of an angular feature in $f(\theta)$ or $\frac{d\sigma}{d\Omega}(\theta)$ is $\simeq \frac{1}{l_{cutoff}} = \frac{1}{ka}$ for short range potentials. This is seen in hard sphere scattering, where the forward diffraction peak has a width $\sim \frac{1}{kR}$.

Also, if the Fourier or Legendre coefficients in the expansion of a function fall off exponentially (that is, after $l \gtrsim l_{cutoff}$), then the function $f(\theta)$ being expanded is an analytic fn. of θ. But if the coefficients fall off as a power law, $1/l^p$, then $f(\theta)$ has a discontinuity in one of its derivatives. This discontinuity will occur in the forward direction $(\theta = 0)$.

Now <u>resonance scattering</u>. If the true potential $V(r)$ is attractive, then it may combine with the centrifugal potential (which is always repulsive) to form a curve like this:



That is, to make a well, separated from the asymptotic region by a barrier. Scattering in a potential like this was considered in a homework problem last fall on WKB theory. In that HW problem, it was found that if the energy E is not close to one of the nominal Bohr-Sommerfeld energy levels in the well, then the asymptotic phase shift between incident and reflected waves is determined just by the 1st turning point encountered, that is, r_2 in the diagram, and the well inside makes no difference. But in a narrow range around $E = E_n =$ a BS energy level, the phase shift undergoes a rapid change (as a fn. of energy), increasing by 2π. As we shall now show, this corresponds to the phase shift δ_ℓ increasing by π in a narrow energy range.

Here is a summary of the WKB results. Define regions I to IV as in the diagram. We want to solve the radial Schrödinger eqn,

$$-\frac{\hbar^2}{2m}u''(r) + \left[\frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right]u(r) = E\,u(r),$$

where $E = \frac{\hbar^2 k^2}{2m}$, by WKB theory. We replace $\ell(\ell+1)$ by $(\ell+\frac{1}{2})^2$, which works better for WKB theory of radial equations. We define the radial momentum

$$p(r) = \sqrt{2m\left[E - \frac{(\ell+\frac{1}{2})^2\hbar^2}{2mr^2} - V(r)\right]},$$

which is real in classically allowed regions II and IV, and purely imaginary in regions I and III (the classically forbidden regions). We define

$$S(r,a) = \int_a^r p(r)\,dr \qquad \text{in C.A.R.'s.}$$

$$K(r,b) = \int_b^r |p(r)|\,dr \qquad \text{in C.F.R.'s.}$$

We let

$$\Phi = \frac{1}{\hbar}\oint_{\text{region II}} p\,dr = \frac{2}{\hbar}\int_{r_0}^{r_1} p(r)\,dr = \frac{2}{\hbar}S(r_1,r_0) = \Phi(E)$$

and

kappa

$$\kappa = \frac{1}{\hbar}\int_{r_1}^{r_2} |p(r)|\,dr.$$

Φ is the action in the well II, and κ is the tunneling action. We assume κ is large enough that $e^{\kappa} \gg 1$ and $e^{-\kappa} \ll 1$.

The nominal B-S condition in the well is

$$\Phi(E_n) = (n+1/2)2\pi,$$

defining energies E_n. Note also,

$$\frac{d\Phi}{dE} = \frac{1}{\hbar\omega_{cl}},$$

where ω_{cl} is the classical frequency of oscillation in the well.

Working from left to ~~[illegible]~~ right, we write

$$u_I(r) = \frac{1}{\sqrt{|p(r)|}}\, e^{K(r,r_0)/\hbar}$$

an exponentially growing solution in region I. Then using the connection rules, on coming out into region IV we have

$$u_{IV}(r) = \frac{1}{\sqrt{p(r)}}\left(2e^{\kappa}\cos\frac{\Phi}{2} + \frac{i}{2}e^{-\kappa}\sin\frac{\Phi}{2}\right)e^{i\left[\frac{S(r,r_2)}{\hbar}-\pi/4\right]} + \text{c.c.}$$

The BS condition is $\cos\frac{\Phi}{2}=0$. If E is not close to a BS energy level, then $\cos\Phi/2$ is not small (it is $O(1)$), and the first term $2e^{\kappa}\cos\Phi/2$ dominates over the 2nd term $\frac{i}{2}e^{-\kappa}\sin\Phi/2$. This first term is real, so the phase of the wave $u_{IV}(r)$ in this case is determined by the phase factor $e^{i[S(r,r_2)/\hbar-\pi/4]}$. In fact, neglecting terms of order $e^{-2\kappa}$, the wave is

$$u_{IV}(r) = \text{const.}\times\cos\left[\frac{S(r,r_2)}{\hbar}-\pi/4\right].$$

Here the phase is determined by the particle that comes in from ∞, reflects off t.p. r_2, and returns to ∞. It never sees the well.

Also, the asymptotic form is

$$u_{IV}(r) \underset{r\to\infty}{\sim} \sin(kr - l\pi/2 + \bar{\delta}_l),$$

that is,

$$\frac{S(r,r_2)}{\hbar} - \frac{\pi}{4} \underset{r\to\infty}{\sim} kr - (l+1)\frac{\pi}{2} + \bar{\delta}_l .$$

We write $\bar{\delta}_l$ to distinguish this phase shift from the exact phase shift δ_l, which includes the effect of the potential well. When E is not close to any E_n, then $\bar{\delta}_l \approx \delta_l$, and in fact in many circumstances $\bar{\delta}_l$ is small since the t.p. r_2 is outside the range of the potential.

Now write

$$\left(2\, e^{\kappa} \cos \Phi/2 + \frac{i}{2}\, e^{-\kappa} \sin \Phi/2\right) = \left| 2\, e^{\kappa} \cos \Phi/2 + i/2\, e^{-\kappa} \sin \Phi/2 \right| e^{i \delta_l^{well}},$$

so that

$$\delta_l = \bar{\delta}_l + \delta_l^{well}.$$

As noted, if $\cos \Phi/2$ not small, then $\delta_l^{well} \approx 0$ (the prefactor is nearly real).

But to see what happens near resonance, let

$$E = E_n + \delta E, \quad \text{where } \delta E \text{ is small},$$

so that $\Phi(E) = \Phi(E_n + \delta E) = (n + 1/2) 2\pi + \frac{\delta E}{\hbar \omega_{well}}$.

Then

$$\cos\frac{\Phi}{2} = -(-1)^n \frac{\delta E}{2\hbar\omega_{cl}}$$

$$\sin\frac{\Phi}{2} = (-1)^n ,$$

so $\quad 2e^{\kappa}\cos\frac{\Phi}{2} + \frac{i}{2}e^{-\kappa}\sin\Phi/2$

$$= 2e^{\kappa}(-1)^n\left[-\frac{\delta E}{2\hbar\omega_{cl}} + \frac{i}{4}e^{-2\kappa}\right]$$

Now we see that if $\frac{\delta E}{2\hbar\omega_{cl}} \lesssim e^{-2\kappa}$, then the prefactor becomes nearly pure imaginary, and the phase δ_ℓ^{well} becomes important. In fact, if a complex number $z = |z|e^{i\alpha}$, then $z^* = |z|e^{-i\alpha}$ and

$$\frac{z}{z^*} = e^{2i\alpha}.$$

So here,

$$e^{2i\delta_\ell^{well}} = \frac{-\frac{\delta E}{2\hbar\omega_{cl}} + \frac{i}{4}e^{-2\kappa}}{-\frac{\delta E}{2\hbar\omega_{cl}} - \frac{i}{4}e^{-2\kappa}} = \left(\frac{-\delta E + i\Gamma/2}{-\delta E - i\Gamma/2}\right)$$

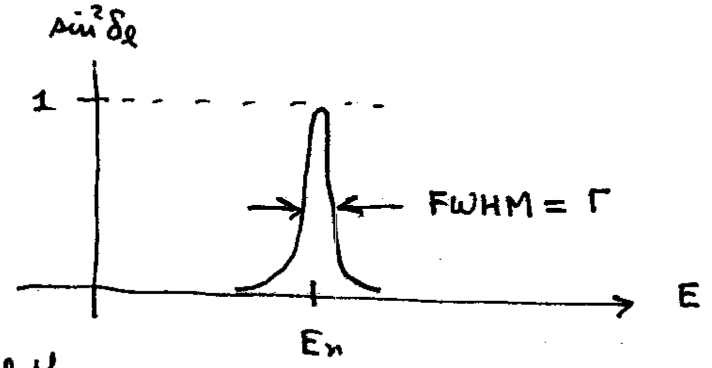
where $\Gamma = \hbar\omega_{cl}\, e^{-2\kappa}$. Notice that $\hbar\omega_{cl}$ is the spacing between the BS energy levels, so $\Gamma \ll$ this spacing.

Now suppose $\bar{\delta}_\ell$ is negligable, so $\delta_\ell = \delta_\ell^{well}$. Then

$$\frac{e^{2i\delta_\ell} - 1}{2i} = \frac{-\Gamma/2}{\delta E + i\Gamma/2} = e^{i\delta_\ell}\sin\delta_\ell .$$

Then $\sin^2\delta_\ell = \dfrac{\Gamma^2/4}{(E-E_n)^2 + \Gamma^2/4}$,

a Lorentzian as a fn. of E,

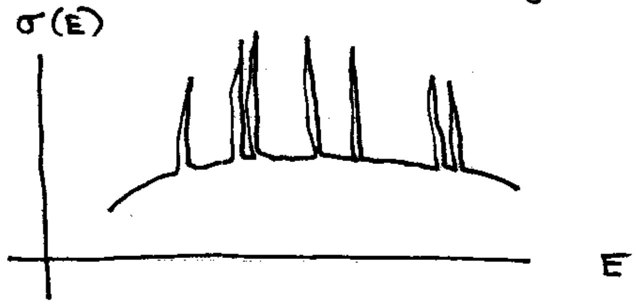


Thus the ℓ-th contribution to the cross section is

$$\sigma_\ell = (2\ell+1)\frac{4\pi}{k^2}\sin^2\delta_\ell,$$

which has the large spike shown at resonance.

These resonances show up as large enhancements in the total cross section, as a fn of E superimposed on a smooth background. They are very common in neutron-nucleus scattering, for example.



like this.

Each resonance corresponds to a definite ℓ value and a definite excitation in the well for a given ℓ.